

OCR (A) Chemistry A-level

Module 4: Core Organic Chemistry

Notes

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11.1 organic chemistry

- Hydrocarbons: a compound containing carbon and hydrogen only
- Saturated: has single bonds only
- Unsaturated: contains carbon-carbon multiple bonds
- Homologous series: a series of organic compounds having the same functional group but with each successive member differing by a CH_2
- Simplest homologous series=alkanes
- Functional group: part of molecule largely responsible for molecule's chemical properties

11.2 nomenclature of organic compounds

- Aliphatic: carbon atoms joined in unbranched/branched chains, or non-aromatic rings
- Acyclic: an aliphatic compound arranged in non-aromatic ring, with/without branches
- Aromatic: some/all carbon atoms found in a benzene ring
- Alkyne: contains at least one triple carbon-carbon bond
- Prefix cyclo- for alicyclic

11.3 representing the formulae of organic compounds

- Molecular formula: shows number of + type of atoms of each element in a molecule e.g. $\text{C}_2\text{H}_6\text{O}$
- Empirical formula: simplest whole number ratio of atoms of each element present in a compound e.g. $\text{C}_4\text{H}_8 \rightarrow \text{CH}_2$
- General formula: simplest algebraic formula for any member of a homologous series
- Displayed formula: shows relative positioning of all the atoms in a molecule and the bonds between them
- Structural formula: uses the smallest amount of detail necessary to show the arrangement of atoms in a molecule

11.4 isomerism

- Structural isomers: compounds with same molecular formula but different structural formula, can have same functional group at different point/different functional group
- Isomers of $\text{C}_{10}\text{H}_{18}\text{O}$ used in perfumes: linalool=lavender smell, geraniol=rose smell

11.5 introduction to reaction mechanisms

- Homolytic fission: each of the covalently bonded atoms takes one of the shared electrons, forms 2 radicals
- Heterolytic fission: one of covalently bonded atoms takes both the electrons, one becomes -ve ion and one becomes +ve ion
- Curly arrows show movement of a pair of electrons
- Addition: two reactants join to make one product
- Substitution: atom or group of atoms is replaced by a different atom/group of atoms
- Elimination: removal of a small molecule from a larger molecule

12.1 properties of the alkanes

- General formula: $\text{C}_n\text{H}_{2n+2}$
- Each carbon is joined to 4 other atoms by single covalent sigma bonds
- Sigma bond: the result of overlapping of 2 orbitals, one from each bonding atom, positioned on line directly between bonding atoms





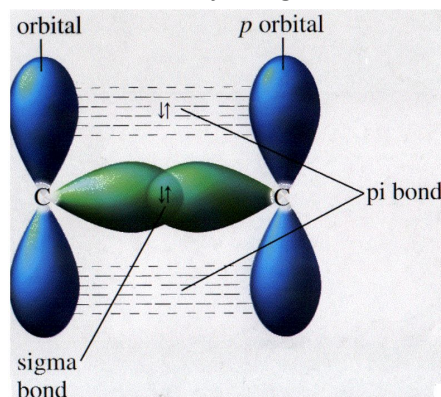
- 3d tetrahedral arrangement around each carbon, 109.5°
- Sigma bonds act as axes around which atoms can rotate freely, so not rigid shape (can change)
- Fractional distillation is used to separate crude oil into fractions
- Increased chain length $\rightarrow$ greater surface area contact $\rightarrow$ stronger London forces $\rightarrow$ higher boiling point
- More branching $\rightarrow$ less surface area contact $\rightarrow$ weaker London forces $\rightarrow$ lower boiling point

12.2 chemical reactions of the alkanes

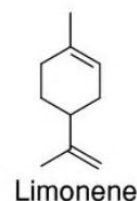
- Not very reactive: C-C/C-H bonds strong, C-C bonds non-polar, C-H bonds can be considered non polar (C and H have similar electronegativities)
- Alkanes are used as fuels because: readily available, easy to transport, burn to release no toxic products
- Carbon monoxide colourless, odourless + highly toxic. Combines irreversibly with haemoglobin in red blood cells to form carboxyhaemoglobin preventing oxygen passing round body. Can turn lips bright pink

13.1 the properties of alkenes

- General formula C_nH_{2n}
- Carbons in double bond have formed three sigma bonds, meaning they have one electron left in a p-orbital, which forms a pi-bond by sideways overlap of 2 p-orbitals. Pi-electron density concentrated above + below line joining nuclei bonded atoms



- Pi-bond locks carbon atoms in position $\rightarrow$ can't rotate
- Trigonal planar shape around double bond, 120°
- Flamingos eat food containing carotenoids. Enzymes in liver convert these to pink/orange pigments deposited in feathers. Beta carotene is related to the chemical that makes carrots orange
- Limonene $C_{10}H_{16}$ is responsible smell/flavour oranges + used in perfumes/cleaning products



13.2 stereoisomerism

- Stereoisomers: have same structural formula but a different arrangement atoms in space
- Fumaric acid (found in wild flower) + maleic acid (from unripe fruit) were the first recognised cis-trans isomers
- Arises because rotation around double bond is restricted + groups attached to each carbon are fixed relative to each other
- For E/Z isomerism, a compound must have: C=C bond & different groups attached to each carbon
- Cis-trans: a type of E/Z isomerism where one of groups on each carbon must be a hydrogen
- Cis=Z, trans=E
- Cahn-ingold-Prelog rules: groups of higher priority same side double bond=Z, groups of higher priority diagonally placed=E. highest priority determined by Mr of atoms attached directly to carbons in double bond (if atom is same, go along chain until 1st different)

13.3 reactivity of alkenes

- More reactive than alkanes: pi bond enthalpy is less so bond is weaker & bond is more exposed as on top/bottom so broken more readily

13.4 electrophilic addition in alkenes

- Double bond in alkene is an area of high electron density due to pi-electrons. High electron density attracts electrophiles
- Electrophile: an electron pair acceptor (usually a +ve ion or a molecule with atom with δ^+ charge)
- Mechanism of electrophilic addition of alkene + hydrogen bromide:
 - Hydrogen bromide is polar and has dipoles because bromine is more electronegative
 - Electron pair in π -bond attracted to δ^+ hydrogen $\rightarrow$ double bond breaks
 - Bond forms between H and carbon atom from double bond
 - H-Br bond breaks by heterolytic fission, electron pair goes to Br
 - Br^- and carbocation formed, they react to form product
- Mechanism for reaction of alkene with Br_2 :
 - Br-Br bond electrons interact w/ π -electrons, causing bond to polarise, inducing δ^+ and δ^- dipoles
 - Electron pair in π bond attracted δ^+ end of $\text{Br}_2 \rightarrow$ bond breaks
 - Bond forms between carbon from double bond & Br
 - Br-Br bond breaks by homolytic fission, electrons go to δ^- end
 - Br^- and carbocation formed, react to make product
- Markownikoff's rule: tertiary carbocations most stable, primary least stable (because alkyl groups push electrons towards +ve charge, charge spread over alkyl groups. More groups=more spread charge). Classified by number of R groups on +ve carbon. Major product is one where H attaches to carbon with most H's attached directly.

13.5 polymerisation in alkenes

- Prefix poly used to name monomer
- N shown before reactant & after square brackets at bottom for product
- Poly(ethene) used in supermarket bags, bottles + toys. Depending on manufacturing method, different densities can be made w/ different structures, properties + uses. High density has linear chains, low density has branched chains (flexible)



- Poly(chloroethene) can be made flexible/rigid, used for: pipes, sheeting + insulation cables
- Poly(propene) used for: toys, guttering, windows etc
- Poly(phenylethane): packaging material/food trays + cups
- Poly(tetrafluoroethene): coating non-stick pans, cable insulation
- Lack of reactivity → challenge for disposal since most are non-biodegradable
- Recycling: conserves fossil fuels + decreases waste going in landfill. Have to be sorted by type, chopped into flakes, washed, dried, melted then cut into pellets + used to make new products
- Disposal/recycling PVC hazardous due to high chlorine content + range additives. Putting them in landfill is not sustainable & when burnt they release HCl (corrosive) + other toxic gases. New tech uses solvents to dissolve polymer, precipitates PVC from solvent, solvent can then be re-used
- Some are difficult to recycle, but have a high stored energy value so can be incinerated to produce heat, generating steam to turn turbine to produce electricity
- Feedstock recycling: chemical + thermal processes to reclaim monomers, gases or oil from waste polymers. Can be used as raw materials for production of new polymers. Key advantage: able to handle unsorted/unwashed polymers
- Bioplastics: produced from plant starch, cellulose, plant oils + proteins- renewable & sustainable (protects environment & conserves oil reserves)
- Biodegradable polymers: broken down by microorganisms into water, carbon dioxide + biological compounds. Can be used as bin liners for food waste so both compost
- Photodegradable polymers: (oil based) contain bonds weakened by absorbing light to start degradation OR light absorbing additives used

14.1 properties of alcohols

- Compared to alkanes: less volatile (hydrogen bonds must be overcome for alcohol to become a gas, these are stronger than London forces in alkanes), higher melting point (hydrogen bonds), greater water solubility (alkanes non-polar so can't form hydrogen bonds with water, alcohols can so are more soluble). Differences become much smaller as carbon chain length increases
- Alkanes have non-polar bonds because H/C electronegativity is very similar, molecules are non-polar, weak London forces. Alcohols have polar O-H bond because of difference in electronegativity, molecules are polar, have weak London forces and hydrogen bonds
- Alcohols can be used to de-ice cars because when mixed with ice, it decreases the melting point dramatically
- Classified as primary/secondary/tertiary depending on the number of alkyl groups attached to C with OH group

14.2 reactions of alcohols

- As number of carbons in alcohol chain increases, quantity heat produced per mol increases when burnt

15.1 chemistry of the haloalkanes

- Nucleophile: an electron pair donor
- Carbon has δ^+ charge and can attract nucleophiles, which replace the halogen
- Hydrolysis: a chemical reaction involving water/aq solution of a hydroxide causing breaking of a bond in a molecule
- Mechanism hydrolysis:



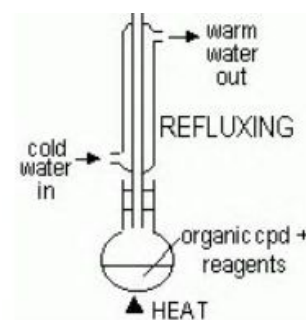
- OH⁻ (nucleophile) approaches C from opposite side to halogen (minimises repulsion)
 - Lone pair on OH attracted & donated to δ⁺ C, forming bond
 - Carbon-halogen bond breaks by heterolytic fission
- Rate of hydrolysis increases as strength of the carbon-halogen bond decreases, C-I fastest
- Measuring rate hydrolysis in primary haloalkanes:
 - Set up 3 test tubes of 1cm³ ethanol and couple drops of 1-chloro/bromo/iodo butane
 - Put in water bath at 60°C & place a test tube with silver nitrate in. Allow to reach constant temp
 - Add 1cm³ silver nitrate to each test tube quickly + start stop watch
 - Observe time taken for ppt to form (white/cream/yellow)

15.2 organohalogen compounds in the environment

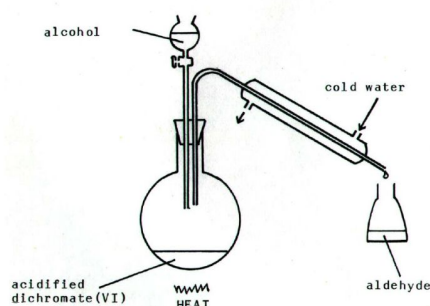
- Ozone layer: outer edge earth's stratosphere. Absorbs UV-B radiation from sun's rays, depletion ozone → increased genetic damage + greater risk skin cancer. Continually formed + broke down by UV: 1st O₂ → 2O, then steady state set up where rate formation is same as rate broken down O₂ + O ⇌ O₃
- CFC's remain stable until they reach the stratosphere. UV breaks carbon-halogen bond by homolytic fission to form radicals. Photodissociation: radiation initiating break down e.g. CF₂Cl₂ → CF₂Cl• + Cl•
- Break down of ozone:
 - Propagation 1: Cl• + O₃ → ClO• + O₂
 - Propagation 2: ClO• + O → Cl• + O₂
 - Overall: O₃ + O → 2O₂
 - Chlorine radical can go on in chain reaction, breaking down 1000s molecules
- Other radicals: NO formed by lightning strikes + air travel:
 - NO• + O₃ → NO₂• + O₂
 - NO₂• + O → NO• + O₂
 - Overall O₃ + O → O₂
 - Research into alternatives to CFC's → coolants using hydrocarbons, ammonia or CO₂ & pump-action spray dispensers being produced. Organobromine compounds are under close scrutiny as it is suspected they release toxins that may interfere w/ endocrine system in humans

16.1 practical techniques in organic chemistry

- Basic set quick fit apparatus: round bottom/pear shaped flask, receiver, screw-tap adaptor, condenser, still head
- Heating under reflux:
 - to prepare organic solid without boiling off solvent, reactants or products
 - water bath can be used rather than Bunsen if can be carried out below 100°C
 - heating mantle can be used so no naked flame, which is safer if apparatus leaks/cracks
 - anti-bumping granules added to liquid so boils smoothly (otherwise large bubbles at bottom → glassware vibrates + jumps)
 - glass joints greased lightly so apparatus comes apart easily after experiment
 - condensers should be clamped loosely- outer jacket is very fragile



- never put stopper in top- closed system so pressure would build up & it would explode
- distillation:
 - method to separate a pure liquid from its impurities
 - glass joints greased lightly so apparatus comes apart easily after experiment
 - flask used to collect distillate so is not airtight



- purifying organic products: if you can't tell which is the organic layer, add water to see which layer gets bigger. Then use a separating funnel:
 - ensure tap is closed, pour in mixture, place stopper in top + invert to mix
 - allow layers to settle (+ add water if unsure which is which)
 - place conical flask under, remove stopper + open tap until whole lower layer has left
 - collect other layer in second conical flask
- acid impurities can be removed by adding aqueous sodium carbonate & shaking in separating funnel. CO_2 will be produced, so turn upside down + open tap to stop pressure building. Then remove aq layer sodium carbonate + wash with water, then run layers into separate flasks
- drying an organic product:
 - a drying agent is an anhydrous inorganic salt that readily takes up water to become hydrated (CaCl_2 (hydrocarbons), CaSO_4 , MgSO_4)
 - add organic liquid to conical flask + add some drying agent w/ spatula + swirl
 - place stopper on to prevent product evaporating + leave for 10mins
 - if solid stuck in clump, it means water is present so add more drying agent until it becomes a fine powder
 - decant liquid into another flask (if dry it should be clear)
- re-distillation: sample may still contain impurities because organic liquids have close boiling points. Carry out second distillation, collecting product with exact boiling point (narrower range=purer product)

17.1 mass spectrometry

- detects mass to charge ratio of molecular ion giving molecular mass of compound
- molecular ion peak is peak furthest to right. Could be $M+1$ peak due to carbon-13 isotope
- fragmentation: molecular ions break down into fragment ion and a radical (radicals are uncharged so not detected)
- used in drug testing in sport e.g. clenbuterol is considered performance enhancing drug

17.2 infrared spectroscopy

- covalent bonds have energy + vibrate naturally around central point, increasing with increasing temperature



- absorbing IR causes them to bend/stretch more. Amount this happens depends on mass of atoms (heavier vibrate slower) & strength of bond (stronger vibrate faster)
- use wavenumber scale- proportional to frequency
- using infrared spec to identify molecules:
 - sample placed in IR spectrometer
 - beam IR radiation $200-4000\text{ cm}^{-1}$ passed through
 - molecules absorb some IR + emerging beam is analysed to identify frequencies absorbed
 - IR spec is usually connected to a computer that plots a graph of transmittance against wavenumber
- Fingerprint region: region below 1500 cm^{-1} with unique peaks to identify particular molecule
- Water vapour, carbon dioxide + methane absorb longer frequency IR from sun because it's the same frequency as the natural frequency of their bonds. Re-emit energy as radiation, increasing the temperature of the atmosphere close to earth service → global warming
- All organic compounds produce a peak $2850-3100$ from C-H bond
- Applications: remote sensors analyse IR spectra vehicle emissions to detect pollutants & IR-based breathalysers pass beam IR through breath + detect IR absorbance, detecting characteristic ethanol bonds (more absorbed, higher reading, more ethanol in breath)

